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ARL 63-63

DEPARTURES FROM LTE IN EMISSION AND ABSORPTION BY CONTINUOUS ENERGY STATES

I. RADIATIVE EQUILIBRIUM

LUDWIG OSTER

YALE UNIVERSITY OBSERVATORY
NEW HAVEN, CONNECTICUT

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FOREWORD

This interim technical report was prepared by the Yale University Observatory, New Haven, Connecticut on Contract AF 33(657)-7271 for the Aeronautical Research Laboratories, Office of Aerospace Research, United States Air Force. The research reported herein was accomplished on Task 7073-01, "High Energy Generation and Control" of Project 7073, "Research on Plasma Dynamics under the Technical Cognizance of Dr. W.G. Braun of the Plasma Physics Research Laboratory of ARL.

ABSTRACT

A general formulation of the theory of departures from LTE in free-free emissions and absorption is developed. The problem is treated subject to the restrictions to steady state and radiative interactions. Particle distribution function and radiation field are studies separately, special attention is given to the transfer problem. The possibility of negative absorption (maser action) is discussed.

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1. INTRODUCTION

The importance of departures from local thermodynamic equilibrium (LTE) was first recognized in connection with certain astrophysical problems, in particular, in connection with the interpretation of the spectrum of the outer solar atmosphere¹. Stellar plasmas are, in the observable layers, rather weakly ionized, so that the major part of the radiation spectrum consists of spectral lines, i. e., emissions and absorptions involving only bound states, with the free energy states in LTE. In physical terms this statement implies that the free energy states of the electrons are distributed according to a Maxwellian distribution, whereas emission and absorption are connected by Kirchhoff's law².

In many domains of laboratory physics, however, plasmas are completely ionized, and the population of bound states can be altogether neglected. Then, only the free electrons are involved in radiative interactions, and departures from a Maxwellian distribution of the free energy states.

The purpose of this paper is to outline a general formulation of departures from LTE in free-free emissions and absorptions. In this report, we restrict our considerations to steady states, where the change in the population of states is (during observation times) small compared with the populations themselves, and to radiative transitions which involve emission or absorption of a single photon.

Radiative interactions affect the particle distribution and the spectrum of the radiation field. There are therefore always two sets of conditions to be considered, derived from the behavior of the radiation field, and from the behavior of the particles. Neglecting one set of conditions does mathematically not lead

to any contradiction, but leads to physically invalid solutions. This fact has been pointed out previously³.

We begin by deriving the steady state condition for the particle distribution function (Section 2), turning to the radiation field in Section 3. In Section 4, the trivial solution (LTE) is discussed. Section 5 deals with some obvious physical consequences of the steady-state condition, Section 6 contains a discussion of the relations between particle distribution function and local intensity of the radiation field. In an Appendix, the question of possible maser action involving continuous transitions is discussed.

2. STEADY-STATE CONDITION FOR THE ENERGY DISTRIBUTION OF FREE PARTICLES

If a steady state has been reached in a plasma, the number of particles entering a certain energy state must equal the number of particles leaving that state. This relation then holds for all energy states.

Consider an arbitrary state with energy E_0 , populated by $N(E_0) dE_0$ particles per unit volume. Neglecting non-radiative transitions, the following processes will occur: the particle may absorb a quantum

•

$$\Omega = n\omega \quad (1)$$

from the incident radiation field and move up to the energy level

$$E_1 = E_0 + \Omega, \quad (2)$$

or it may emit a quantum Ω , descending to the energy level

$$E_2 = E_0 - \Omega. \quad (3)$$

The number of these processes per unit time depends on the interaction mechanisms (bremsstrahlung, cyclotron radiation, Cerenkov radiation, etc.), on the local intensity of the radiation field (absorption and induced emission only), and on the number of particles $N(E)$ available.

The pertinent quantities were defined and discussed in detail in a previous publication². We recall that the number of particles in the energy range $E, E+dE$ has the dimension $[N(E) dE] = \text{cm}^{-3}$, so that the LTE - distribution (Maxwell distribution) reads

$$N(E) dE = 4 \pi N_0 \frac{1}{2} (\pi K T)^{-3/2} e^{-E/KT} e^{\frac{1}{2}} dE. \quad (4)$$

Writing the radiation field too in terms of energies (Ω) instead of angular frequencies (ω), we have $[I_\Omega d\Omega] = \text{erg/cm}^2 \text{ sec sterad}$, so that in LTE (Planckian distribution)

$$I_\Omega d\Omega = B_\Omega d\Omega = \frac{\Omega^3}{4 \pi^3 n^3 c^2} [e^{\Omega/KT} - 1]^{-1} d\Omega. \quad (5)$$

Later on, the abbreviation

$$H_0 = 4 \pi^3 n^3 c^2 [\text{erg}^3 \text{ cm}^2 \text{ sec sterad}] \quad (6)$$

will be used.

The relations between the cross sections of spontaneous emission, absorption and induced emission read²

$$Q_{in} = \frac{H_0}{\Omega^3} Q_{sp}$$

and

$$Q_{ab} = \frac{H_o}{\Omega^3} \sqrt{\frac{E}{E-\Omega}} Q_{sp} . \quad (8)$$

In the following,

$$Q(E, \Omega) \equiv Q_{sp} , \quad (9)$$

where $E = m v^2/2$ is the energy of the upper state from which the spontaneous emission takes place. The probability coefficient Q then has such a dimension that $[Q(E, \Omega) d\Omega] = \text{sec}^{-1} \text{ sterad}^{-1}$.

We are now ready to write down the number of incoming (n_+) and outgoing (n_-) processes for the arbitrary energy state E_0 :

$$n_+ = \int_0^\infty N(E_0 + \Omega) Q(E_0 + \Omega, \Omega) \left[1 + \frac{H_o}{\Omega^3} I_\Omega \right] d\Omega + \\ + \int_0^{E_0} N(E_0 - \Omega) Q(E_0, \Omega) \sqrt{\frac{E_0}{E_0 - \Omega}} \frac{H_o}{\Omega^3} I_\Omega d\Omega , \quad (10)$$

and

$$n_- = \int_0^\infty N(E_0) Q(E_0 + \Omega, \Omega) \sqrt{\frac{E_0 + \Omega}{E_0}} \frac{H_o}{\Omega^3} I_\Omega d\Omega + \\ + \int_0^{E_0} N(E_0) Q(E_0, \Omega) \left[1 + \frac{H_o}{\Omega^3} I_\Omega \right] d\Omega . \quad (11)$$

In steady state,

$$n_- = n_+, \quad (12)$$

or, after some algebra,

$$\int_0^\infty Q(E_0 + \Omega, \Omega) \{ E_0 + \Omega, \Omega \} d\Omega = \int_0^{E_0} Q(E_0, \Omega) \{ E_0, \Omega \} d\Omega. \quad (13)$$

The bracket symbol is defined by the following expression

$$\{ x, y \} = N(x) + I_y \frac{H_0}{y^3} [N(x) - \sqrt{\frac{x}{x-y}} N(x-y)]. \quad (14)$$

In physical terms, $Q(E_0, \Omega)$. $\{ E_0, \Omega \}$ represents the difference (positive or negative) between the number of absorption processes (upwards) and emission processes (downwards) involving the states E_0 and $E_0 - \Omega$. Clearly, if the states E_0 and $E_0 - \Omega$ are in detailed balancing (LTE), the bracket is zero.

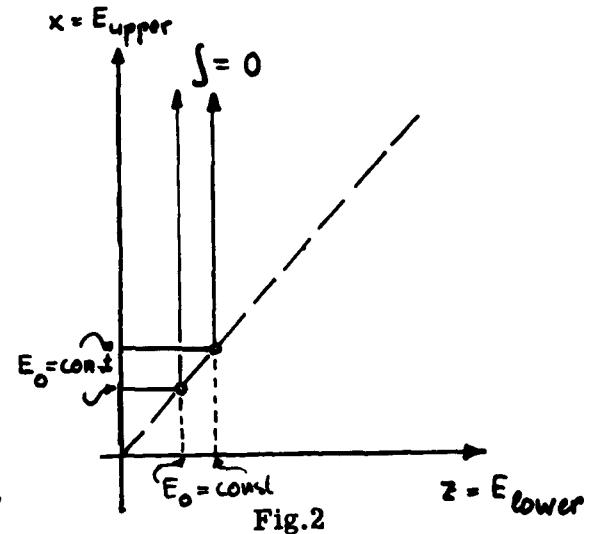
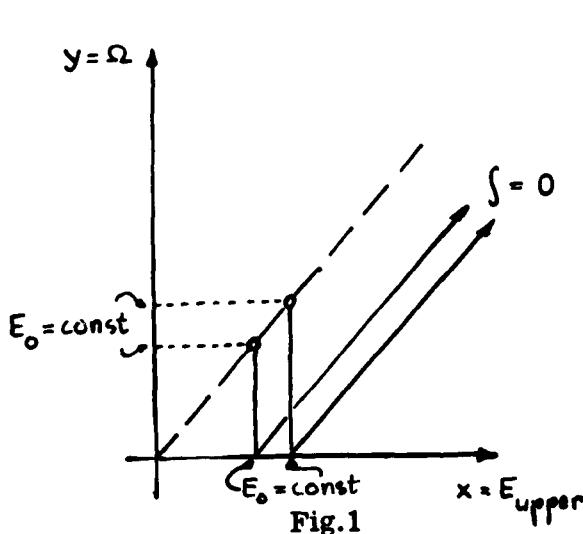
The intensity of the local radiation field can always be expressed, for a given photon energy Ω , in terms of a Planckian with a pseudo-temperature T . Similarly, the number-density of particles in two states differing in energy $\Delta E = \Omega$ can be expressed in terms of a Maxwellian distribution, with a fixed total number N_0 of particles and, again, a pseudo-temperature T' . If the bracket $\{ E_0, \Omega \}$ is zero, $T = T'$. It will be shown later that the situation where $\{ E_0, \Omega \} = 0$ for all Ω is equivalent to LTE.

Returning to the general discussion, we write the steady-state condition (13) in the following form:

$$\int_0^{\infty} Q(x, y) \cdot \{x, y\} \cdot dy \Big|_{x = E_0 + y} = \int_0^{E_0} Q(x, y) \cdot \{x, y\} \cdot dy \Big|_{x = E_0}, \quad (15)$$

for all $E_0 = \text{const.}$

Mathematically, the steady-state condition can be visualized in the following way: over the x - y plane, the function $Q(x, y)$. $\{x, y\}$ may be plotted. The steady-state condition (15) then requires that along ALL paths outlined in Fig 1, the integral must vanish.



Let us finally rewrite Eq. (15) in terms of $x = E_{\text{upper}}$ and $z = E_{\text{lower}}$ instead of x and y , where x , y and z are related by

$$x - z = y. \quad (16)$$

The result reads

$$\frac{\infty}{E_0} \int Q(x, x-z) \cdot \{x, x-z\} dx \Big|_{z=E_0} + \int_0^{E_0} Q(x, x-z) \cdot \{x, x-z\} dz \Big|_{x=E_0} \quad (17)$$

The graphic representation similar to Fig 1 is outlined in Fig 2, where now the function

$$Q(x, x-z) \cdot \{x, x-z\} = f(x, z) \quad (18)$$

must be plotted vs. x and z.

3. STEADY-STATE CONDITION FOR THE RADIATION FIELD

Before we discuss the steady-state condition for the particles, Eq. (17), any further, let us briefly glance at the conditions which a stationary state imposes on the radiation field. So far, the radiation field entered our description only through I_Ω as a parameter in the bracket function $\{x, y\}$. We shall see presently that in order to conserve radiative energy, only a considerably weaker condition must be satisfied, but that self-consistent solutions to any given problem are subject to a set of additional requirements, outlined in Section 6.

There are two characteristic differences between the radiation field and the particle distribution. First, the particles are stationary, whereas the radiation field consists of photons entering and leaving a certain volume element. Second, the number of particles before and after a radiative interaction is conserved in steady state, whereas the number of photons may increase or decrease as a result of these radiative interactions. In fact, a typical problem in radiation theory is the flow of radiation through a plasma in which the total radiative energy is of course conserved, but in which the high energy photons, for example, are

broken up into several low energy units.

Hence, the only condition imposed on the radiation field under stationary conditions is that the total radiative energy at each point is conserved. This quantity is found by multiplying the number of transitions involving a state E_0 by the appropriate energy Ω , and then integrating over all states E_0 from 0 to ∞ , i.e., by forming

$$\int_0^\infty dz \int_z^\infty dx \cdot f^*(x, z) = \int_0^\infty dE_x \int_0^x dz \cdot f^*(x, z) = 0, \quad (19)$$

where now

$$f^*(x, z) = (x - z) Q(x, x-z) \{ x, x-z \} \quad . \quad (20)$$

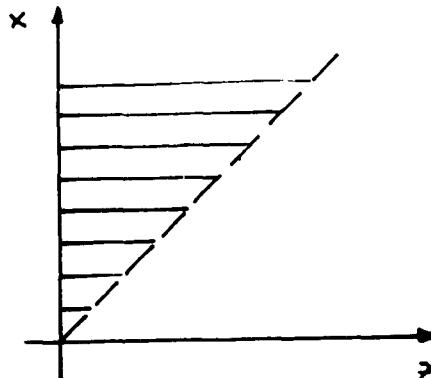


Fig.3

Mathematically, the two representations (19) correspond to the two possible orders of integration in Cartesian coordinates of the function $f^*(x, z)$ over the shaded area in Fig 3. The equality of integrals of this type is shown in texts on analysis, for instance, in Jeffrey's book⁴. Identifying $f^*(x, z)$ with his $f(y)$, our coordinates x and z with Jeffrey's x and y , and letting his $t \rightarrow \infty$ [f^* clearly

vanishes at infinity on physical grounds] , transforms our expressions (19) into Jeffrey's standard equations.

In physical terms the first integral (19) corresponds to counting first all transitions leading into a fixed lower level E_o , and then varying E_o (or z) over the whole range, whereas the second integral in (19) first counts all transitions leading into a fixed upper state E_o , and then varies this upper state E_o (or x) from 0 to ∞ .

The steady-state condition for the radiation field is clearly weaker than the condition for the particle distribution, Eq. (17), since it involves only the INTEGRAL over expressions of the type (17). It will, therefore, in general not restrict the validity of solutions compatible with (17). However, the energy condition (19) is not redundant in the sense that it is automatically fulfilled for all solutions to (17), due to the additional factor $(x-z)$ under the integral.

Finally, self-consistency of solutions imposes a set of conditions developed in the context of the transfer problem in Section 6.

4. TRIVIAL SOLUTION: LTE

Before we discuss condition (17) in more detail, the existence of a trivial solution should be mentioned. This trivial solution corresponds to $f(x, y) \equiv 0$ everywhere. On physical grounds, this means

$$\{ x, x-z \} = 0 \quad \text{for all } x, z, \quad (21)$$

since a Q which vanishes everywhere implies no radiative interactions whatsoever. Eq. (21) describes detailed balancing for all energies and energy differences. Intuitively it is obvious that detailed balancing can only occur in LTE. To show

that the two concepts are equivalent under very general conditions requires, however, a considerable amount of statistical mechanics, and is far beyond the scope of this paper⁵. We shall merely VERIFY that for radiative transitions between continuous energy states detailed balancing and LTE are equivalent.

That LTE is SUFFICIENT for detailed balancing is obvious: inserting a Maxwellian distribution for $N(E)$ and a Planck function for I_Ω makes the bracket symbol (14) vanish identically, i.e., leads to detailed balancing.

Reflection is needed to show that LTE is NECESSARY for detailed balancing.

For this purpose, we write Eq. (14),

$$\left\{ x, y \right\} = N(x) + I_y \frac{H_0}{y^3} \left[N(x) - \sqrt{\frac{x}{x-y}} N(x-y) \right] \equiv 0, \quad (22)$$

in the form

$$\frac{N(x-y)}{\sqrt{x-y}} = K(y) \frac{N(x)}{\sqrt{x}}, \quad (23)$$

where

$$K(y) = \frac{y^3}{H_0 I_y} + 1 \quad (24)$$

does not depend on x . Using the further abbreviation

$$G(t) = N(t) / \sqrt{t}, \quad (25)$$

we have the functional equation

$$G(x-y) = K(y) G(x). \quad (26)$$

We now expand $K(y)$ around $y = 0$,

$$K(y) = K(0) + \frac{dK}{dy} \Big|_{y=0} \cdot y + \dots, \quad (27)$$

with

$$K(0) = 1, \quad (28)$$

Because of Eq. (26),

$$\left[\frac{dK}{dy} \right]_{y=0} = K'_0 \quad (29)$$

cannot vanish in general, since $N(x)$ must contain the Maxwellian distribution for which obviously $K'_0 \neq 0$. In fact, it can be shown that if $K'_0 = 0$, the normalization integral

$$\int_0^\infty N(E) E^n dE = N_0 \langle E^n \rangle \quad (30)$$

diverges, corresponding to an infinite temperature (see below).

Next, we expand $G(x-y)$ around x ,

$$G(x-y) = G(x) + \frac{dG}{dx} \cdot y + \dots \quad (31)$$

For $y \rightarrow 0$ we find from Eqs. (26), (27) and (31)

$$G(x) - \frac{dG}{dx} y = [1 + K'_0 \cdot y] G(x), \quad (32)$$

with the solution

$$G(x) = \text{const.} e^{-K'_0 \cdot x}, \quad (33)$$

or

$$N(E) dE = \text{const.} e^{-K'_0 \cdot E} \cdot \sqrt{E} \cdot dE. \quad (34)$$

Eq. (34) represents the Maxwell distribution with

$$K'_0 = 1 / KT. \quad (35)$$

From Eqs. (23) and (24) it is now readily verified that

$$I_\Omega \cdot \frac{H_0}{\Omega^3} = [e^{+K'_0 \cdot \Omega} - 1]^{-1}, \quad (36)$$

which is the Planckian distribution with the same value (35) for K'_o . Hence, we have verified that the condition $\{x, y\} = 0$ is equivalent to LTE.

5. DISCUSSION OF THE STEADY-STATE CONDITION FOR PARTICLES

We return now to the general steady-state condition for particles, Eq. (17), with the additional condition (19) representing conservation of radiative energy. A detailed discussion of sufficient and necessary conditions to be satisfied by I_Ω and $N(E)$ in order to be compatible with Eqs. (17) and (19) will be given in a later report. It suffices here to mention certain MINIMUM requirements concerning the bracket function (14).

Since the bracket function must vanish integrated along ALL paths of the type outlined in Fig 2, there is necessarily at least one point on EACH integration path for which

$$\{x, x-z\} = 0 . \quad (37)$$

All these points form a one-dimensional continuum which from obvious geometrical considerations falls in either one of the two categories:

1. All z -values, $0 \leq z \leq \infty$, fulfill Eq. (37). The corresponding x -values lie in a range $x_o \leq x \leq \infty$ with $x_o > 0$, finite. Similarly, the corresponding y -range will not, in general, comprise all possible values.
2. All $y \equiv x-z$ values, $0 \leq y \leq \infty$, fulfill Eq. (37). $x \geq x_o$, $0 \leq z \leq z_o$; $x_o > 0$, $z_o > 0$.

Figs 4 and 5 illustrate schematically the two cases. As emphasized before, these are minimum requirements, and whether in an actual case there exists one of the

outlined minimum solutions will depend on the form of $Q(E, \Omega)$.

Fig.4. Case 1.

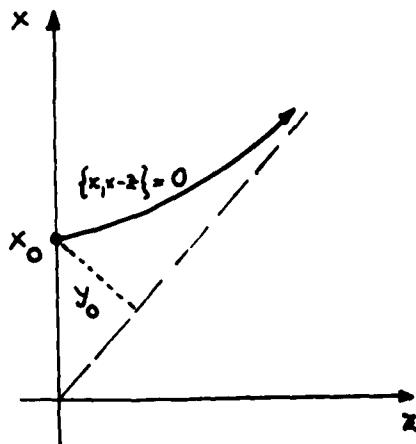
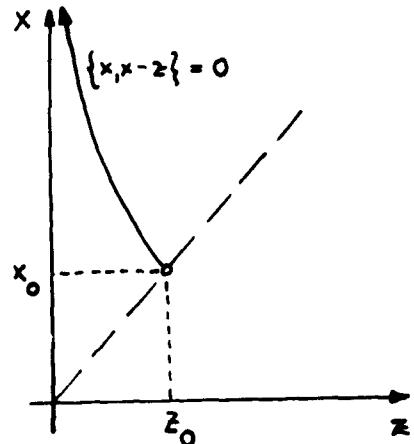


Fig.5. Case 2.



Assuming a solution of the type illustrated in Fig 5, we find that I_{Ω} can be represented by a Planckian function with a temperature $T(\Omega)$ which may depend on $\Omega \equiv y$. At the same time, the ratio $N(E + \Omega)/N(E)$ can be represented for all E -values by a Maxwellian distribution with the same $T(\Omega)$ -value from above. Only if T is independent of Ω in the whole plane, thus $\{x, z\} \equiv 0$, we come back to the LTE-solution.

6. RADIATIVE TRANSFER AND STEADY STATE

So far, I_{Ω} and $N(E)$ were treated as independent quantities. This procedure, however, is in general not permitted. In fact, in most practical cases, I_{Ω} is the sum of all contributions to the emission from the whole plasma surrounding the specific point under discussion. The emission itself, on the other hand, depends on $N(E)$.

There are numerous cases one might think of which range from the completely self-consistent problem, in which I_{Ω} is SOLELY due to the plasma radiation, to the opposite extreme, where I_{Ω} contains practically only OUTSIDE radiation. The general problem is described by the transfer equation which under steady-state conditions reads²

$$dI_{\Omega}/d\tau_{\Omega} = S_{\Omega} - I_{\Omega} , \quad (38)$$

and has the solution

$$I_{\Omega} = \int_{\Omega}^{\infty} S_{\Omega}(\tau_{\Omega}) e^{-\tau_{\Omega}} d\tau_{\Omega} \quad (39)$$

The optical depth is defined for Eq (39) so that at the plasma point under study. The integration is extended to infinity, i. e., to the plasma boundary. Any incoming radiation field at this boundary can then be accounted for by a properly matched source term S_{Ω} . I_{Ω} depends, of course, on direction through

$$d\tau_{\Omega} = \kappa_{\Omega} ds , \quad (40)$$

where s is an arbitrary spatial coordinate, κ_{Ω} is the absorption coefficient.

In our present terminology, the emission coefficient

$$\epsilon_{\Omega} = \Omega \int_{\Omega}^{\infty} Q(E, \Omega) \cdot N(E) \cdot dE \Big|_{\Omega = \text{const}} , \quad (41)$$

so that the dimension of ϵ_{Ω} is $\text{erg/cm}^3 \text{ sec sterad}$. Next,

$$\kappa_{\Omega} = \frac{H_{\Omega}}{\Omega^3} \cdot \Omega \cdot \int_{\Omega}^{\infty} Q(E, \Omega) \left[\sqrt{\frac{E}{E-\Omega}} N(E, \Omega) - N(E) \right] dE \Big|_{\Omega = \text{const}} \quad (42)$$

(dimension: cm^{-1}). From Eqs (41) and (42), the source function

$$S_{\Omega} = \epsilon_{\Omega} / \kappa_{\Omega} [\text{cm}^{-2} \text{ sec}^{-1} \text{ sterad}^{-1}] \quad (43)$$

follows immediately.

Hence, in order to obtain a self-consistent solution, I_{Ω} should be replaced in Eqs (17) and (19), i.e., in the bracket function, by the appropriate solution (39) to the transfer problem, using Eqs (41) - (43) to represent the source function. The result is then a set of integral equations that contain solely $N(E)$ as unknown.

It should be emphasized that I_{Ω} cannot be simply replaced by S_{Ω}^3 . Such a procedure corresponds to what may be called "semi-detailed" balancing, implying

$$\tau_{\Omega} = \infty , \quad (44)$$

because of Eq (39), or

$$\epsilon_{\Omega} = \infty I_{\Omega} . \quad (45)$$

With the aid of Eqs. (41) - (43), Eq (45) can be written as

$$\begin{aligned} & \int_{\Omega}^{\infty} Q(E, \Omega) \cdot N(E) \cdot dE \Big|_{\Omega = \text{const}} = \\ & = \frac{H_0}{\Omega^3} I_{\Omega} \int_{\Omega}^{\infty} Q(E, \Omega) \left[\sqrt{\frac{E}{E-\Omega}} N(E-\Omega) - N(E) \right] dE \Big|_{\Omega = \text{const}} , \end{aligned} \quad (46)$$

or, in our previous terminology, as

$$\int_{\Omega}^{\infty} Q(x, y) \cdot \{ x, y \} \cdot dx \Big|_{y = x-z = \text{const}} \quad (47)$$

for all $\Omega \equiv y$. The path of integration is illustrated in Fig 6.

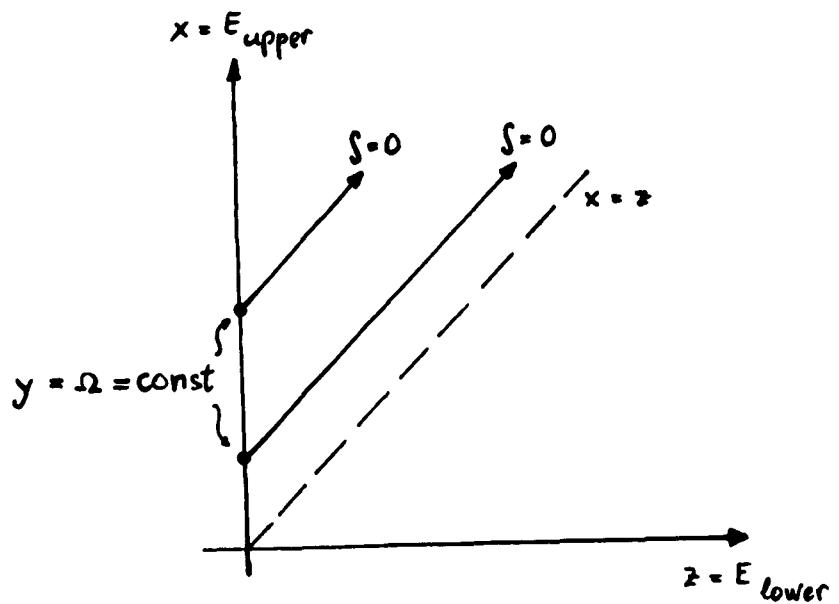


Fig.6

This additional condition will in general be compatible with Eq (17) only for
 $\{x, y\} \equiv 0$, i.e., in LTE.

ACKNOWLEDGEMENT

The mathematical derivations outlined in Section 4 were obtained in collaboration with Mr. R. Goldman, of this Laboratory.

APPENDIX: MASER TYPE AMPLIFICATION

Our definition (42) allows for a very elementary discussion in general terms of the problem of possible negative absorption, i.e., maser-type amplification of continuous radiation. This problem has recently been treated by several authors in view of possible applications⁶.

Since the factor in front of the integral is positive, the problem of negative χ_Ω 's reduces to the study of

$$\int_{\Omega}^{E_m} Q(E, \Omega) \left[\sqrt{\frac{E}{E-\Omega}} N(E-\Omega) - N(E) \right] dE \approx R(E_m) - R(\Omega) \quad (48)$$

In (48) the infinite upper limit is replaced by a formal cut-off parameter E_m in order to ensure finite normalization for strongly non-Maxwellian distribution functions. Negative absorption occurs, if

$$|R(E_m)| < |R(\Omega)|. \quad (49)$$

The inequality (49) can, theoretically, be fulfilled in two cases: since Q on physical grounds is always positive, only the slope as a function of E is of importance. On the other hand, slope AND sign must be taken into account in the case of the bracket $[]$. In fact, for a distribution of the mathematical form of the Maxwell distribution, Eq (4), $[]$ goes through zero for $T \rightarrow \infty$, and becomes negative for formally negative values of T .

Since all known interaction mechanisms lead to transition probabilities that effectively increase with increasing E , a combination of

$$[] < 0, Q \underset{-|n|}{\not\propto} E \quad (50)$$

is of little practical interest. Hence, negative absorption is confined to hypothetical distribution functions whose energy variation is of the form

$$N(E) \underset{\delta > 0}{\not\propto} E^{\frac{1}{2} + \delta}, \quad (51)$$

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